­­­Multi-stage model predictive control of agricultural anaerobic digestion plant with uncertain substrate characterization

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# Highlights

* Demand-oriented operation of AD process despite uncertain influent concentrations
* Model predictive control (MPC) for optimization of substrate feedings
* Multi-stage MPC control satisfies operational limits of gas storage filling levels
* Time-variant setpoints of methane production are tracked and disturbances rejected
* Orthogonal collocation enables fast computation for real-time application of MPC

# Graphical Abstract

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# Abstract

Revenues of anaerobic digestion (AD) plants can be increased by generating biogas and electricity on demand or through biogas upgrading. However, suitable control procedures for individual applications are required to guarantee optimal process conditions. Moreover, substrate characterization at full scale plants is often subject to large uncertainties. In this contribution, a multi-stage nonlinear model predictive controller (NMPC) was designed to optimize substrate feedings under uncertain substrate characterization. Simulations demonstrate that multi-stage NMPC provides biogas on demand to flexibly operate a combined heat and power unit, while save gas storage filling limits are ensured (20% safety margin) despite uncertain influent concentrations. Additionally, multi-stage NMPC successfully tracked changing setpoints of constant methane production for biogas upgrading within 12 h, and rejected disturbances posed by disturbing feedings of very high uncertainty. By exemplifying demand-oriented operation of AD plants despite uncertain substrate characterization, this study showcases ecologically and economically sustainable strategies for AD plant operation.

*Keywords:* Biogas Technology, ADM1, Robust Control, Influent Uncertainty, Flexibilization, Gas Storage, Demand-oriented operation

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# Introduction

To achieve the United Nations’ ambitious goals of the Paris agreement and shift towards renewable energy sources, anaerobic digestion (AD) plays an important role in ensuring electricity grid stability (Purkus et al., 2018). Unlike wind and solar energy, power generated from biogas through AD is not dependent on fluctuating weather conditions. Instead, the AD process can produce and buffer biogas for demand-oriented generation of sustainable electricity and heat (Theuerl et al., 2019).

To remain competitive with other renewable energy sources, AD plants must adopt innovative strategies to increase revenues and lower operational costs, especially as state subsidies are fading out (Daniel‐Gromke et al., 2018). To this end, three promising strategies are (i) demand-oriented cogeneration of power and heat, (ii) biogas upgrading to biomethane, and (iii) flexibility to utilize alternative substrates (Mauky et al., 2016; Daniel‐Gromke et al., 2018; Theuerl et al., 2019).

In demand-oriented cogeneration, biogas is converted to electricity during peak load times, offering higher selling prices but also entailing high investment costs (Purkus et al., 2018). This is conventionally pursued by increasing installed capacities of combined heat and power (CHP) units and gas storage (GS) volumes. Alternatively, demand-oriented feed optimization optimally controls the amount and composition of utilized substrates. Thereby, biogas and electricity production can be aligned with anticipated electricity prices, which reduces the need for additional GS capacities (Mauky et al., 2016). Yet, to accurately predict biogas production and the nonlinear behavior of the AD process, reliable process models and input characterization are required.

The second strategy is to equip existing AD plants with biogas upgrading units to produce biomethane for direct injection into the natural gas grid, which is increasingly pursued internationally (Schmid et al., 2019). Since biogas upgrading units typically operate under stationary conditions for optimal efficiency, biogas production must typically be maintained at constant setpoints despite variable feedstocks (Jønson et al., 2022) .

The third strategy lies in reducing substrate costs and utilizing low-cost feedstocks, such as organic waste or agricultural residues (Daniel‐Gromke et al., 2018; Theuerl et al., 2019). While for the majority of biogenic feedstocks, there already exist profitable value chains in Germany, there is still ample unused potential for use in AD plants (Steindl et al., 2025).

All three strategies require robust control schemes to ensure optimal process performance and stable operating conditions despite uncertain substrate characterization. Moreover, predictive control of AD necessitates reliable process models and sound knowledge of substrate characterization. While there exist sophisticated AD models, such as the well-established Anaerobic Digestion Model No. 1 (ADM1) proposed by Batstone et al. (2002) and its extensions (Kegl et al., 2025), their application to control studies is limited due to the numerous model parameters that need to be calibrated, and scarcely available data at full scale plants to do so (Segura et al., 2025). Instead, Bernard et al. (2001) proposed a model explicitly designed for monitoring and control. Due to lower system order and fewer parameters, this model has been successfully applied to monitoring and control of AD processes in lab- and pilot scale (García-Sandoval et al., 2016; Raeyatdoost et al., 2023). However, the semi-empirical model proposed by Bernard et al. (2001) lacks a clear stoichiometry foundation (compared to the ADM1) and is based on chemical oxygen demand (COD), typically applied for process characterization in wastewater engineering. Therefore, Weinrich and Nelles (2021) systematically simplified the ADM1 by summarizing degradation pathways and converting it from COD to mass-based reference unit. This simplification eased deployment in agricultural settings and has been validated in different lab and full scale settings (Tisocco et al., 2024; Weinrich et al., 2021).

A critical aspect of AD modeling is to reliably estimate influent concentrations of nutrients and organic compounds. This depends on accurate substrate characterization (Jimenez et al., 2015; Lübken et al., 2015) and involves extensive laboratory measurements (Liebetrau and Pfeiffer, 2020). Furthermore, the anaerobically degradable part of influent concentrations needs to be estimated, because not all organic material is degradable under anaerobic conditions, such as lignin (Lübken et al., 2015). One established way to quantify anaerobic degradability is by assessing the substrate's biochemical methane potential (BMP) through batch experiments (Dandikas et al., 2018; Koch et al., 2020). However, in practice, BMP measurements are subject to significant measurement errors (Hafner et al., 2020). Moreover, in full scale AD operation, time-consuming batch experiments are often omitted in favor of literature values of comparable substrates. While nutrient compositions of common agricultural substrates are well-documented (especially for energy crop silages and manure) (Fisgativa et al., 2020; Lübken et al., 2015), there still exists substantial variation in anaerobic degradability across individual samples and seasons (Weinrich et al., 2018). In this study, uncertain influent concentrations are thus modeled as a consequence of underlying measurement uncertainties. These uncertainties diminish the confidence in resulting model inputs and lead to unreliable simulation results (Gehring et al., 2013; Tisocco et al., 2024). In the model-based feed control of AD, these uncertainties can potentially lead to process instability (Kegl et al., 2025). To this end, robust model-based control approaches explicitly consider these uncertainties to safeguard operational constraints, such as GS limitations.

There exist numerous approaches in the literature to control the AD process (Gaida et al., 2017). Many of them have been applied to wastewater treatment plants (Alcaraz-González et al., 2021; Méndez-Acosta et al., 2008). In the context of agricultural AD plants, one powerful approach is model predictive control (MPC). MPC was originally developed in the petrochemical industry in the 1970s, and is valued for its intuitive concept and ability to handle nonlinear models and constraints on states and inputs (Qin and Badgwell, 2003). Hence, it has since been applied to a wide range of applications (Mayne, 2014), including biological systems (Kim et al., 2023) and AD (Körber et al., 2022). Mauky et al. (2016) proposed a nominal MPC scheme for demand-oriented CHP operation of an agricultural AD plant, and validated it experimentally in pilot and full scale. However, their process model did not include process inhibition, and their MPC disregarded model uncertainties.

At the core of MPC lies the process model, which serves to predict the future system behavior. To this end, nominal MPC does not explicitly consider model uncertainties. However, since each model is only an approximation of reality, real-world applications usually face a plant-model mismatch (Qin and Badgwell, 2003). Compared to nominal MPC, this mismatch is explicitly addressed in advanced MPC schemes, e.g., robust or min-max MPC (Piceno-Díaz et al., 2020), stochastic MPC (Mesbah et al., 2014) or tube-based MPC (Guo et al., 2024). When dealing with a parametric plant-model mismatch (i.e., assuming a structurally suitable model), multi-stage MPC, as proposed by Lucia et al. (2013), offers a promising solution. It has been successfully demonstrated in multiple applications, such as polymerization and penicillin production, and is accessible as the open-source Python library *do-mpc* provided by Fiedler et al. (2023).

The present study investigates the performance of multistage MPC for robust and dynamic operation of AD plants in the presence of uncertain substrate characterization. For this purpose, the AD process was modeled by a simplified ADM1 which includes process inhibition, and was applied in a simulative case study covering biogas upgrading. Additionally, the AD model was augmented by a GS model and applied in a second case study covering cogeneration with a CHP unit. In different operational configurations, the system performance was assessed, as well as the satisfaction of constraints imposed by the capacity limits of the GS. This study thereby illustrates the capabilities of model-based feed control for more competitive AD operation and underscores the importance of explicitly considering uncertainties of substrate characterization.

# Materials and methods

## 2.1 Dynamic AD model: ADM1-R3

Due to the complexity of the original ADM1 (Batstone et al., 2002) with 34 states and 52 model parameters, the present study applied the mass-based simplification ADM1-R3 proposed by Weinrich and Nelles (2021). The ADM1-R3 describes the AD process in two steps: (i) a combination of hydrolysis, acidogenesis, and acetogenesis, and (ii) methanogenesis. Characteristic model equations are described in Hellmann et al. (2023). In the present study, the model was slightly extended by splitting carbohydrates (CH) into two fractions of slowly and fast degradable CH, and , with corresponding hydrolysis constants and . The influent CH were allocated to the fast and slow fraction through an additional fraction parameter . The model involves 18 states and 27 model parameters, cf. Tab. 1 and supplementary information (SI). The setup of the AD model is illustrated in Fig. 1e.

### 2.1.1 Gas storage model

The ADM1-R3 was extended by a model of the GS and a CHP unit. The operating schedule of the CHP unit was taken from Mauky et al. (2016) and is shown in Fig. 1b. In accordance with Dittmer et al. (2022), the GS was modeled as a membrane enclosure with a variable volume, which is connected to a fixed-roof AD digester of constant liquid and headspace volumes and . Isobaric conditions at a slightly elevated pressure of 1.014 bar were assumed within the GS. Further, a constant elevated temperature of 50 °C (Stur et al., 2022) was assumed as a conservative estimate of the GS capacity during the summer months with high sun radiation.

The GS was assumed to be homogeneously filled with biogas from the AD digester (CH4, CO2 and H2O, all modeled as ideal gases). It is depleted through the CHP unit, whose thermal power supply is given through its electrical capacity and efficiency , as well as the lower heating value (LHV) of CH4. Two additional states and describe the volume of CH4 and CO2 in the GS. Corresponding model equations of the GS are derived in the SI. Fig. 1c shows a qualitative dynamic course of the GS filling level. Numerical values of all introduced model parameters are summarized in Tab. 1.

### 2.1.2 AD plant dimensioning

Dimensions of the AD plant, GS and CHP unit were inspired by the research biogas plant at the German Biomass Research Center (Deutsches Biomasseforschungszentrum, DBFZ) as reported in Mauky et al. (2016) and summarized in Tab. 1. The CHP unit was assumed to have an electrical capacity of 50 kW and an electrical efficiency of 36%. To obtain a ratio between CHP unit and GS capacity in the range of Dittmer et al. (2022), the maximum GS capacity was set to 280 m³.

## 2.2 Uncertain substrate characterization

There exist analytical laboratory procedures to determine raw macronutrients of CH, proteins (PR) and lipids (LI) (Liebetrau and Pfeiffer, 2020). However, their anaerobic degradability can only be quantified heuristically, e.g. through batch tests (Jimenez et al., 2015). Therefore, in this study, the influent macronutrients CH, PR and LI were considered as uncertain since the ADM1-R3 only considers the anaerobically degradable shares of raw macronutrients (Weinrich et al., 2021). Other

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| **Table 1:** Model parameters of ADa, b process, CHPa unit and GSa, c, as well as nominal values and variation coefficients required for substrate characterization and uncertainty quantification of macronutrients. |
| |  |  |  |  |  |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | | Category | Variable | | Value | Unit | | Category | | Variable | | Value | | Unit | | | Operational AD parametersa, c |  | | 163 | m³ | | Substrate feeding | |  | | 80 | | m3 d-1 | | |  | | 16.3 | m³ | |  | | 450 | | m3 d-1 | | |  | | 311 | K | |  | | 1000 | | kg m-3 | | |  | | 1.013 | bar | | Kinetic parametersb | |  | | 2.5 | | d-1 | | | Gas Storagea, c |  | | 280 | m3 | |  | | 0.25 | | d-1 | | |  | | 50 | °C | |  | | 0.4 | | - | | |  | | 1.014 | bar | |  | | 0.2 | | d-1 | | |  | | 518.4 | J kg-1 K-1 | |  | | 0.1 | | d-1 | | | CHP unita, c |  | | 50 | kW | |  | | 0.02 | | d-1 | | |  | | 36 | % | |  | | 0.4 | | d-1 | | |  | | 50.01 | MJ kg-1 | |  | | 0.14 | | kg m-3 | | | Substrate/VCa, f | | BMPa, d  [L kg-1 VS] | | | TSa, e  [% FM] | | a, e  [% TS] | | a, e  [% TS] | | a, e  [% TS] | | a, e  [-] | | Maize silage (MS) | | 357 | | | 33.73 | | 4.43 | | 7.81 | | 2.44 | | 50 | | Grass silage (GrS) | | 372 | | | 31.74 | | 11.29 | | 13.93 | | 2.14 | | 5 | | Sugar beet silage (SBS) | | 389 | | | 39.27 | | 9.39 | | 3.39 | | 0.19 | | 3 | | Cattle manure (CM) | | 246 | | | 8.08 | | 23.65 | | 16.63 | | 2.38 | | 24 | | VC [%]f | | 14.51 | | | 1.94 | | 7.40 | | 5.52 | | 10.04 | | - | |
| a AD: anaerobic digestion, CHP: combined heat and power, GS: gas storage, VC: variation coefficient, BMP: biochemical methane potential, TS: total solids, : measurements of raw ash, protein and lipids, VS: volatile solids, FM: fresh matter, : number of samples.  b The first three kinetic parameters of the ADM1-R3 differ from those in Weinrich and Nelles (2021), the other kinetic parameters are given only for the sake of completeness.  c Individual values were inspired by the research biogas plant at DBFZ described in Mauky et al. (2016).  d BMP of sugar beet silage taken from Heidarzadeh Vazifehkhoran et al. (2016), all others are based on in-house measurements at DBFZ, which have been assessed in triplicates.  e Nominal values of TS, , , were determined from in-house substrate characterization at DBFZ with given sample size.  f VC of BMP taken as mean residual standard deviation of all four substrates in Hafner et al. (2020), Tab. 3, excluding cellulose. VC of , , , and were taken from Delory et al. (2025). |

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| **Figure 1**: Setup and components of the simulated system: **(a)** AD process and controller (constant methane production); as well as AD process, gas storage, CHP unit and controller (cogeneration); **(b)** CHP operating schedule; **(c)** schematic course of the resulting GS filling level; **(d)** block diagram of controller, estimator and plant/simulator; the second simulator is used for sensitivity analysis (based on nominal influent concentrations); **(e)** block diagram of the ADM1-R3 model components. |

parametric or structural uncertainties were ignored. The following typical agricultural AD   
substrates were considered (Ahmed et al., 2016; Segura et al., 2025; Hahn et al., 2014): grass silage (GrS), maize silage (MS), sugar beet silage (SBS) and cattle manure (CM). Individual substrate costs per t of fresh matter (FM) are provided in Tab. 2.

### 2.2.1 Nominal computation

ADM1-R3 influent concentrations, denoted as , were computed according to Delory et al. (2025). To compute individual concentrations of dissociated components of acetic acids, carbon dioxide and ammonia nitrogen typical pH values for silages and manure were taken from Weißbach (Weißbach and Strubelt, 2008a, 2008b, 2008c) and Fisgativa et al. (2020), respectively.

Total solids () were assumed to consist of crude ash and crude macronutrients (crude carbohydrates, crude proteins and crude lipids), where crude CH include lignin. Crude values are given in percentage of , therefore it holds (Weinrich et al., 2021)

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|  |  | (2.1) |

Influent concentrations of degradable macronutrients can be computed based on crude macronutrients, their corresponding degradability quotient , , and the mass density of FM (Lübken et al., 2015), where the latter was assumed as 1000 kg m-3 for all substrates

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|  |  | (2.2) |

PR and LI were considered fully degradable, i.e. (Lübken et al., 2015), thus all non-degradable macronutrients were attributed to CH. This is considered sufficiently accurate for the investigated agricultural substrates due to their low LI and PR concentrations, cf. Tab. 1. The degradability of CH was derived from the total degradability of individual substrates

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|  |  | (2.3) |

To this end, total degradabilities were estimated by the ratio of substrates’ observed BMP and the stoichiometric BMP for agricultural substrates of 420 L kg-1 of degradable volatile solids (DVS) (Weißbach, 2009). Resulting ADM1-R3 influent concentrations are provided in the SI.

### 2.2.2 Linear uncertainty propagation

In this study, uncertainties of influent macronutrients were derived from uncertainties of the underlying laboratory measurements by applying linear uncertainty propagation (Ku, 1966). This

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| **Table 2:** Parameters of MPC problems for case study 1 and 2. |
| |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | | Category | Variable | | Value | | | Unit | | Substrate costsa | Maize silage (MS) | | 45 | | | € t-1 FM | | Grass silage (GrS) | | 31 | | | € t-1 FM | | Sugar beet silage (SBS) | | 52 | | | € t-1 FM | | Cattle manure (CM) | | 5 | | | € t-1 FM | | MPC parameters |  | Case study 1b | | | Case study 2c |  | |  |  | | 28 | 28 (14) | d | |  |  | | 0.5 | 0.5 | h | |  |  | | 15 | 48 | - | |  |  | | 1 | 1 | - | |  |  | | 1.5 (1) | 1 (2) | - | |  |  | | 1E3 | 1E3 (1E2) | - | |  |  | | 1 (0.1) | 100 | - | |  |  | | - | 50 (60) | % | | Disturbance feedingd | Time window | 5-10, 13-17, 22-26 | | | 5-7, 9-12, 15-19 | d | | Volume flow | 0.58, 1.16, 1.74 | | | | m3 d-1 | | Additional OLR | 1, 2, 3 | | | | kg VS m-3 d-1 | |
| a Individual values were estimated based on experience from DBFZ in consideration of Hahn et al. (2014). For all silages, a 30% cost increase was considered due to inflation since 2014.  b Differing values used for sensitivity analysis are given in parentheses.  c Differing values used for comparison between nominal and robust MPC are given in parentheses.  d Only applies for setpoint tracking of constant methane production and cogeneration (Sec. 3.3.1 and 3.3.2) |

allows to compute the standard deviation (SD) of a variable which is a function of independently distributed variables , i.e. , as

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|  |  | (2.4) |

With (2.2) and (2.3), SDs of influent macronutrients are propagated as

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|  |  | (2.5) |
|  |  | (2.6) |
|  |  | (2.7) |

SDs were based on variation coefficients and nominal values of individual substrates, which are both summarized in Tab. 1. Resulting SDs of influent macronutrients are provided in the SI.

## 2.3 Model predictive control

MPC is an advanced model-based control approach that optimizes system performance by using a mathematical model to predict the system’s behavior over a future time horizon (Qin and Badgwell, 2003). This horizon is divided into equidistant time intervals, during which inputs (here substrate volume flows) are commonly assumed to be constant. The interaction between the controller, the plant, and an estimator is shown in Fig. 1d. At each time step, the MPC solves an optimal control problem (OCP), which delivers the optimal input trajectory for the entire prediction horizon. Only the first entry of the input trajectory is applied to the plant (or a simulator). Afterwards, the horizon is shifted forward by one time step, and the OCP is re-initialized with updated estimates of the process state based on the latest measurements . This is known as the receding horizon approach.

### 2.3.1 Multi-stage nonlinear model predictive control

Multi-stage nonlinear MPC is a control scheme aimed at robust controller performance with respect to parametric model uncertainties (Lucia et al., 2013). The core of this method is the creation of a scenario tree in which all explicitly defined uncertainty realizations are combined with each other (Fig. 1d and Fig. 2). Creation of individual branches is repeated at each time step until a specified robust horizon , after which the branches maintain constant values until the end of the prediction horizon. Multi-stage MPC then minimizes the weighted sum of the cost functions across all scenarios in the scenario tree. In this study, each scenario was weighted equally, reflecting equal probabilities of all scenarios.

### 2.3.2 Simplified scenario tree design for AD model

Lucia and Engell (2014) stated that constraint satisfaction can only be guaranteed if parametric uncertainties assume the discrete values considered in the scenario tree. Yet they reported that even for nonlinear systems, scenario tree design with upper and lower uncertainty limits often leads to constraint satisfaction for all possible uncertainty realizations within these limits.

In this study, only macronutrient inlet concentrations were considered uncertain. While these uncertainties are on a continuous scale in real life (dotted line within the plant block in Fig. 1d), it often suffices to consider a limited number of uncertainty realizations (Lucia et al., 2013). These realizations were modeled as positive or negative deviations from their nominal values, while the deviations were chosen as a certain number of SDs based on the underlying uncertainty propagation, as shown in Fig. 2 (right).

Four substrates were considered for this study. Since each of them contained three macronutrients (CH, PR, LI), this would result in 12 discrete uncertain values. Even for robust horizons of 1 this would lead to different multi-stage scenarios, which was deemed computationally infeasible. Instead, in a first step, the uncertain values for all macronutrients were grouped and varied simultaneously for all substrates. This led to a total of different multi-stage scenarios and is illustrated in Fig. 2 (left). Sensitivity analysis (cf. Sec. 3.2), though, showed that the most significant influence on model predictions was caused by uncertain influent CH. Therefore, the scenario tree was reduced to two scenarios as illustrated in Fig. 2 (right).

Robust horizons larger than one were not applied due to the scenario tree’s exponential growth and associated computational demand (Lucia et al., 2013), and by assuming uncertainty realizations as unknown but approximately time-invariant across the prediction horizon (Fig. 2).

## 2.4 Case studies

Two case studies were considered in this investigation, shown as two different pathways in Fig. 1a. Case study 1 addresses constant methane production through the AD process for subsequent biogas upgrading and feed-in into the natural gas grid. In practical applications, this

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| **Figure 2**: Scenario trees with grouping of uncertain macronutrients for all substrates (left) and with only two possible uncertain values for influent carbohydrates (right) as well as robust and prediction horizons. |

requires to separate CO2 from the generated biogas in a biogas upgrading unit, which is not   
modeled here. Since biogas upgrading processes are typically run at steady state (Jønson et al., 2022), the aim was to track piecewise constant setpoints of methane flow rate. Case study 2 considers cogeneration with a CHP unit and a GS for buffering, whose filling levels must remain within safe operational limits. Both case studies were investigated with and without disturbances, which model the feeding of a large amount of highly uncertain substrate (case study 1 and 2) as well as GS measurement noise (case study 2 only).

### 2.4.1 Constant methane production (case study 1)

The ADM1-R3 was used without an additional GS and simulated for a total of 28 days (4 weeks). Four different setpoints of methane volume flow were imposed at days 0, 3, 6 and 9. The setpoints were heuristically chosen as 350, 550, 450 and 350 m3 CH4 d-1. The MPC was not informed on upcoming setpoint changes, which reflects that in real-life scenarios non-foreseeable setpoint changes may suddenly be required.

In the framework of MPC, case study 1 was modeled through a cost function which penalizes squared normalized deviations between the realized () and required () methane production across the prediction horizon of length as shown in Eq. (2.8). Furthermore, the feed volume flow of substrates (system input ) is incorporated to incentivize economic substrate usage. Their total amount is penalized proportionally to their respective cost, where denotes the number of substrates. Both linear and quadratic input weighting were tested, with quadratic weighting delivering significantly smoother setpoint tracking during initial tests. Moreover, the squared changes of substrate feed volume flow are penalized to prevent the controller from acting too erratically. Otherwise, initial trials showed that this erratic controller behavior led to deep pH drops, from which the AD process would not recover. To consider the individual cost function components in similar orders of magnitude, they were normalized to their setpoint and maximum substrate cost, as described in Eq. (2.8) and (2.9) respectively.

The AD model equations were discretized by orthogonal collocation on finite elements (OCFE, cf. Sec. 2.5) and denoted as discretized dynamic and measurement equations and . Enforcing positive states through non-negativity constraints proved to be unnecessary during initial tests, which was thus omitted. Normalized inputs were constrained between 0 and 1. The cost function for a single multi-stage scenario and the resulting OCP are shown in Eq. (2.8) and (2.9). Tab. 2 summarizes required coefficients and hyperparameters used for case study 1.

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|  |  | (2.8) |
|  |  | (2.9) |

### 2.4.2 Cogeneration (case study 2)

Case study 2 addresses demand-oriented cogeneration. For this purpose, the ADM1-R3 was augmented by the GS model described in Sec. 2.1. Since CHP units typically have an operation point of optimal electrical efficiency, the CHP unit was assumed to be either turned on at 100% capacity or turned off. A weekly CHP operating schedule inspired by Mauky et al. (2016) was repeated for a total of 30 days, as illustrated in Fig. 1b.

To keep the GS filling level within the specified bounds, the cost function (2.10) penalizes the squared deviation between the actual filling level and a constant setpoint level (Mauky et al., 2016). Initial tests revealed good results for filling level setpoints just below 50%. The normalized GS filling level was computed from the sum of its individual normalized components, i.e. the GS states and , as well as (cf. Sec. 2.5.3). A linear substrate cost term was added for the same reason as in case study 1. Initial tests showed no necessity to penalize the rate of input changes, nor for a terminal cost, which were thus omitted.

Constraints to the OCP are posed by the system equations. The ODE system contains two additional equations due to the GS states, which were constrained to be non-negative. The normalized GS filling level was further soft-constrained between 5% and 95% by adding slack variables and (Fiedler et al., 2023). Eq. (2.10) and (2.11) show cost function and constraints of a single multi-stage scenario. Tab. 2 summarizes the parameters used for case study 2.

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|  | (2.10) |
|  | (2.11) |

### 2.4.3 Modeled disturbances

#### 2.4.3.1 Disturbance feeding

The first of two modeled disturbances, called disturbance feeding, addresses the following context. Operational cost of AD plants can be reduced by feeding low-cost substrates, such as manure or organic residues (Daniel‐Gromke et al., 2018), which might only be available irregularly and in small amounts. Conducting detailed substrate characterizations for such additional substrates might therefore not be economically viable, resulting in higher uncertainties than for regular substrates. Therefore, occasional dosages of cattle manure with 2.5 times the regular SDs were added, acting as a fixed and known disturbance to the controller at specified times and flow rates. Tab. 2 summarizes volume flow rates, resulting additional organic loading rates (OLRs) and time windows of the simulated disturbance feedings. OLRs are based on nominal cattle manure.

#### 2.4.3.2 Gas storage measurement noise

For case study 2 an additional noise was imposed on the GS states. This aims to reflect measurement noise of the GS filling level, which typically suffers from low accuracy and resolution (Stur et al., 2022). At every time step both GS states were independently imposed with a random uniform noise of ±1% of the respective GS state. Additionally, every five hours the magnitude of this noise was increased to ±3%.

## 2.5 Numerical implementation

### 2.5.1 Orthogonal collocation on finite elements

The *do-mpc* toolbox used in this study requires the model ODEs to be discretized at equidistant time steps of the prediction horizon (Fiedler et al., 2023). For this purpose, orthogonal collocation on finite elements (OCFE) was used (Finlayson, 1980). This method divides continuous time into discrete elements and approximates the ODE solutions with polynomial trial functions. Accuracy is ensured via predefined collocation points within the finite elements. This converts the differential equations into a set of algebraic equations which depend on the trial function parameters. Their solution delivers the system trajectory and thus replaces the ODE integration.

For simulations in this study, a time step of 0.5 h was used with one finite element per time step. A Gauss-Radau collocation scheme of order 2 was applied (Biegler, 2010).

### 2.5.2 Initialization of simulations

All dynamic MPC simulations were preceded by a 500 d open loop simulation to achieve a steady-state. During open loop simulation, a constant mix of all four substrates was fed continuously, consisting of 0.64 m3 d-1 of each silage and 1.92 m3 d-1 of cattle manure. Based on nominal substrate characterization, this resulted in a steady-state OLR of 4 kg VS m-3 d-1.

### 2.5.3 Normalization

To improve numerical stability of the MPC, states and inputs were normalized. All 18 AD states and influent concentrations of the extended ADM1-R3 were normalized to their maximum absolute value observed during the preceding steady-state simulation. Both GS states and were normalized to the total GS volume . Substrate feed inputs were normalized to the maximum feeding values assumed for the respective conveyor augers or pumps, which operate differently for solid and liquid substrates, as illustrated in Tab. 1 (Substrate feeding).

### 2.5.4 Normalized root mean squared error

The error between two signals and of the same length is quantified by means of the normalized root mean squared error (NRMSE)

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|  | , with mean value . | (2.12) |

### 2.5.5 Soft- and hardware

Multi-stage MPC was implemented in *do-mpc* (Fiedler et al., 2023), version 4.6.4. Note that in *do-mpc*, control and prediction horizon have the same length. As a nonlinear solver, *ipopt* (Wächter and Biegler, 2006) was used, which was accelerated by embedding the linear solver *MA27* of the coin-HSL library. All procedures were implemented in Python 3.10.12. Simulations were run on a MacBook pro (macOS Sequoia 15, Apple M1 chip, 8 GB of RAM).

# Results and discussion

## 3.1 Distributions of substrate characterization

Individual influent macronutrient concentrations were obtained for each substrate based on substrate data available at DBFZ and nominal calculations. These are illustrated as boxplots in Fig. 3 with individual sample sizes in the legend. Additionally, normal distributions based on linear uncertainty propagation of measurement errors are shown. Distributions are discussed with respect to nominal (mean) values; this is followed by resulting error bands, both theoretical and measured, based on linear uncertainty propagation and measurement data, respectively.

Clearly, CH form the largest macronutrient fraction, which holds for silages (by an order of magnitude), but also for manure. All substrates distinctly differ in CH and PR. SBS exceeds all other substrates in CH but is very low in PR and LI, which is well in line with the literature (Ahmed et al., 2016; Kryvoruchko et al., 2009). CM is generally low in all macronutrients compared to silages (Segura et al., 2025), and is only undercut by SBS in PR and LI. GrS is relatively high in LI, followed by MS, which has also been observed by Ahmed et al. (2016).

The theoretical CH uncertainty is the smallest for CM despite the large sample size. This can be attributed to the generally low macronutrient concentrations due to its high water content (Tab. 1). For CH, the theoretical uncertainty delivers SDs of similar orders of magnitude for all three silages in the range of 36-50 g L-1. CH of CM, by comparison, only show a SD of around 5 g L-1. For PR and LI, small theoretical SDs were obtained for all macronutrients with a range of 0.5-2.5 g L-1 for PR and 0.06-0.82 g L-1 for LI.

Within the investigated substrate samples, the results for CM compare well among boxplots and normal distributions, both for mean values and error bands. For SBS, mean and median of SBS differ substantially for CH and PR, which may suggest an outlier among the small sample size of 3. Nevertheless, measured error bands are estimated well by linear error propagation, especially for LI, with little underestimation for CH and PR. For MS and GrS, the theoretical and measured error bands of PR are in the same range with SDs of 1.5-3 g L-1. Linear error propagation, however, underestimates the measured LI error bands in MS and GrS.

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| **Figure 3**: Theoretical and measured distributions of degradable fractions of macronutrients. Theoretical distributions are shown by means of gaussian curves, measured distributions by means of boxplots. Sample sizes used for measured distributions are provided in the legend. Note that y-axes only apply for theoretical distributions. |

In the literature, a wide spectrum of substrate characterizations is reported for comparable substrates. This holds especially true for degradable macronutrient concentrations due to the manifold ways to derive them (Koch et al., 2020; Lübken et al., 2015; Fisgativa et al., 2020). When deriving the ADM1-R3 influent concentrations as described in this study, very similar values are obtained for all silages, e.g. 264, 2.6 and 0.5 g L-1 for CH, PR and LI of SBS (Kryvoruchko et al., 2009), or 204, 28.2 and 10.4 g L-1 for MS, respectively (Ahmed et al., 2016). Fisgativa et al. (2020), conversely, reported higher values for CM with CH, PR and LI in the range of 84, 4 and 5 g L-1. The same authors reported values for MS in a similar range as the present study, whereas PR were stated to be lower and LI higher than in the present study.

In summary, ADM1 influent characterization of comparable agricultural substrates results in starkly different macronutrient values. This is rooted in different breeds of the same substrate as well as seasonal fluctuations, sampling and measurement errors, and different assumptions on degradability (Liebetrau and Pfeiffer, 2020). Linear uncertainty propagation only based on measurement uncertainties results in substantial error bands which realistically reflect observed uncertainties of ADM1 substrate characterization. However, values determined with uncertainty propagation for LI in MS and GrS rather represent lower estimates of measured error bands.

## 3.2 Sensitivity analysis of uncertain macronutrients

The influence of uncertain macronutrient influent concentrations was considered in model simulations according to the block diagram shown in Fig. 1d. Two simulators were run in parallel and provided with the same feed volume flows, but different associated influent concentrations: one with nominal, the other with elevated values (nominal + 1 SD). The first simulator was updated by an ideal estimator (assuming no plant-model mismatch) at each time step, the second one was run in open loop assuming the same feed volume flows. This approach was individually applied for all three macronutrients (CH, PR, LI). Sensitivity analysis is discussed by means of case study 1, while the corresponding controller performance is discussed in Sec. 3.3.1.

Model simulations for nominal and elevated realizations of influent CH, PR and LI concentrations (plotted as dotted and solid lines, respectively) are shown in the SI. Since for the three cases the feed volume flows are almost identical, only those of the first case (differing CH) are shown.

The biggest discrepancy between the two parallel simulations is observed for different values of influent CH, in line with the findings of Donoso-Bravo et al. (2025). This can be explained with the high CH content of used substrates relative to PR and LI, and hence the high absolute values of a single SD. For CH, the two resulting trajectories (nominal vs. elevated) show a NRMSE for methane production of 12410-3 and for pH of 6.110-3. By comparison, varying influent concentrations of PR and LI by 1 SD results in much lower NRMSEs for methane production of 610-3 and 3.210-3 and for pH of 1.610-3 and 3.910-5, respectively.

It was laid out that practical influent uncertainty of LI is underestimated by linear uncertainty propagation. However, even when heavily increasing the number of SDs for LI from 1 to 5, the outcome remains of the same quality: NRMSEs of methane production and pH are 1610-3 and 1.910-4, which is still an order of magnitude lower than for a single SD of CH. Consequently, only CH were considered for constructing multi-stage scenarios due to their high share in macronutrients and corresponding high impact on model predictions. In turn, PR and LI were set constant at their nominal levels, delivering the simplified scenario trees shown in Fig. 2 (right).

## 3.3 Multi-stage MPC performance

### 3.3.1 Setpoint tracking of constant methane production

Fig. 4 shows the controller performance for setpoint tracking of methane production. 1.5 SDs were assumed for influent uncertainty realizations. Plant simulations were based on elevated values of the scenario tree, according to Lucia et al. (2013), and as illustrated in Fig. 1d (Plant block).

The MPC delivers convergence for changing methane production setpoints within less than 12 h and without overshoot, cf. magnifications in Fig. 4. This is achieved by sudden, heavy changes in feedings of manure and silages (top subplot). Feedings are increased for increasing setpoints of methane production and entirely stopped briefly for decreasing setpoints (days 6, 9). Constant setpoints are maintained by quasi-constant substrate feedings after some initial convergence. The hourly OLR varies between 3 and 12, with an average of around 6 kg VS m-3 d-1.

Given the substrate costs in Tab. 2, the optimal substrate composition consists of about equal and nearly constant shares of all substrates, with a slight preference for GrS (cf. magnifications in Fig. 4). When changing the costs of substrates relative to each other, the mix changes in favor of the cheapest silage (plots not shown). However, the methane potential represented by the influent concentrations also affects the substrate mix required to satisfy the setpoint tracking. This explains why SBS has a higher share in feedings than MS although it is more expensive (cf. also Fig. 3).

While co-digestion with constant substrate composition is common in practical AD operation (Hahn et al., 2014), fully continuous feed volume flows are rather uncommon. Instead, quasi steady-state methane production is typically approximated through intermittent substrate dosages in short intervals (Bonk et al., 2018), which leads to fluctuating gas production. Further, a GS was not considered in case study 1 but is usually installed to compensate such fluctuations and ensure constant volume flows, e.g. into an upgrading unit (Jønson et al., 2022). The obtained continuous substrate feeding is, though, a plausible consequence of the OCP formulation, and has also been reported in other simulative studies (Ahmed and Rodríguez, 2020; Kil et al., 2017).

A small permanent tracking error remains especially for the high setpoint (cf. 2nd last subplot in Fig. 4). This is not surprising, as the controller optimizes a cost function that, aside from the tracking error, also considers substrate costs and alternations in feed volume flow, cf. Eq. (2.8). The tracking error can further be decreased by increasing the respective weight in the cost function, i.e. by increasing tuning parameter relative to and/or the substrate costs. This comes at the expense of higher and more erratic feed volume flows (plots not shown).

Disturbance feedings (2nd subplot of Fig. 4) could be rejected well by the NMPC by adequately reducing the feeding especially of silages ahead of time (2nd magnification in top subplot). Note that the controller was informed on upcoming disturbance feedings. The pH could be maintained approximately constant and in a range of 7.2-7.3 and with the most significant drop at the set first setpoint change on day 3. This performance is similar to the one reported by Kil et al. (2017).

The run time for the simulation of 28 d was less than 7 min. This would clearly allow real-time application and underscores the numerical efficiency obtained through orthogonal collocation as discretization and the HSL solver. Overall, the NMPC successfully tracked constant setpoints of methane production with fast convergence and ensured stable process conditions despite disturbance feedings. This required continuous feedings of substrates, which is technically feasible.

### 3.3.2 Save gas storage levels during cogeneration

Controller performance for cogeneration was investigated with an additional GS under disturbance feedings and GS measurement noise. Uncertainty values of controller and plant were chosen as described in Sec. 3.3.1. The dynamic system behavior is shown in Fig. 5 (left) by means of optimal substrate feeds, known disturbance feedings, OLR, GS filling level, gas and methane

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| **Figure 4**: Setpoint tracking performance of methane production for biogas upgrading with disturbance feeding of very uncertain cattle manure. The prediction horizon was 15 time steps (7.5 h). |

production, and pH. The GS filling limits are maintained with a comfortable safety margin of about 20%. Soft constraints on GS filling level at 5 and 95% are shown by grey dashed lines.

The feeding pattern starkly differs from case study 1: instead of continuous feed volume flows, substrates are fed in short, intermittent dosages, which represents a more realistic feeding scenario in full scale (Dittmer et al., 2022). Substrate feeding is dominated by manure, while only in the last

third of the simulation, SBS and GrS are fed, but no MS. The substrate composition changes drastically depending on relative substrate prices. Since CM is by far the cheapest substrate, it is plausible that it is used primarily. Additional parameters influencing the optimal substrate composition are the kinetic constants, especially the hydrolysis constant of CH as the largest macronutrient fraction, and the fraction parameter of influent carbohydrates, cf. Tab. 1.

Feedings mostly lie at the beginnings of CHP on-times, indicated by grey vertical shades. This agrees with Mauky et al. (2016) and underlines the predictive nature of the NMPC: Timely feedings compensate upcoming CHP on-times and thus maintain medium GS filling levels, cf. Eq. (2.10). Likewise, gas production increases sharply with feeding onsets, and then fades out while no substrate is fed (fasting time). While this intermittent feeding is not operational practice in full scale in lieu of quasi steady-state feeding, a time-varying substrate load for flexible AD operation was also reported by Dittmer et al. (2022) or Mauky et al. (2016).

During and after disturbance feedings, ordinary substrate feedings were slowed down, which is plausible as disturbances were assumed to be known to the controller. However, in case of random, unpredicted disturbances with unknown associated uncertainties, disturbance rejection might be less successful, and safety margins of GS filling levels might be slimmer.

Medium hourly OLRs were maintained with an average of around 4 kg VS m-3 d-1. This agrees with values reported by Körber et al. (2022) and those of typical agricultural AD plants (Fachagentur Nachwachsende Rohstoffe e. V., 2021). The share of methane in the produced biogas remains almost constant at around 60%, similar to Körber et al. (2022). Finally, the pH ranges between 7.3 and 7.5, slightly increases at feeding onsets, then drops and recovers during fasting times. pH drops are deeper upon feeding of SBS than of CM, which occurs alongside more pronounced peaks in gas production. Mind the different scales of the y-axis for silages and manure.

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| **Figure 5:** Dynamic gas production for cogeneration with disturbance feeding and gas storage measurement noise under robust MPC with different implementations of process inhibition. On the left, the ADM1-R3 was implemented conventionally with state-dependent process inhibition, while on the right, process inhibition was ignored in both controller and plant model (. The prediction horizon was 48 time steps (24 h). CHP on-times are indicated by grey background shading. | | |

Overall, stable process conditions can be maintained by the NMPC despite flexible feeding of varying substrates and disturbances, which agrees well with the findings of Mauky et al. (2017) and Bonk et al. (2018). Moreover, the controller retains process inhibition at stable levels throughout

the entire simulation, albeit at a low ammonia inhibition factor in the range of 0.25-0.3. The other two inhibition factors of nitrogen limitation and pH inhibition remain at almost 1, rendering them practically inactive (plots not shown). Stable process operation at low levels of ammonia inhibition factors has also been reported by Weinrich et al. (2021) and Wichern et al. (2009). However, multiple different realizations of kinetic parameters (Tab. 1) can describe similar process states, which are hence difficult to distinguish without more detailed investigation or state estimation.

When ignoring the process inhibition, i.e. setting the inhibition factor to 1, the substrate composition changes in favor of manure, and no silages are fed anymore (Fig. 5, right). This is plausible as without inhibition the kinetics of acetoclastic methanogenesis are no longer slowed down, and consequently methane formation is accelerated, well visible in the more spiked gas production and pH fluctuations. Given the much lower substrate cost of manure compared with silages (Tab. 2), the cumulative gas production required to ensure safe GS filling levels can be achieved with manure as a cheaper substrate than silage. Note that the controller was informed on the constant inhibition factor and no further plant-model mismatch was introduced.

In summary, given the hyperparameters in Tab. 1 and 2, the NMPC robustly satisfies constraints on GS filling level through discontinuous substrate feedings predominantly of manure.

## 3.4 Comparison of robust and nominal MPC

Fig. 6. compares the performance of multi-stage MPC (left) and nominal MPC (right) for cogeneration, i.e. with an additional GS, but without disturbance feedings and GS measurement noise. Instead, to challenge the controller performance, uncertainties of influent CH were varied at 2 SDs, and the GS filling level setpoint was increased to 60% (Tab. 2). A total of 14 d (2 weeks) were simulated. Multi-stage scenarios of the robust MPC were based on upper and lower uncertainty values; the plant assumed elevated values as previously (plant block in Fig. 1d), but the nominal MPC was supplied with nominal values of influent CH.

Clearly, nominal MPC (Fig. 6, right) fails to ensure process stability and leads to massive constraint violations of the GS, whereas robust multi-stage MPC (Fig. 6, left) maintains safe GS

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| **Figure 6:** Comparison of robust (left) and nominal MPC (right) in the light of plant-model mismatch during cogeneration without disturbance feeding and GS measurement noise and prediction horizon of 48 time steps (24 h). Controller graphs (index MPC) show 6 h ahead predictions (12 time steps). CHP on-times are indicated by grey background shading. | | |

filling levels and an overall stable process. The reason for the nominal controller’s inferior performance becomes apparent when considering the differences between 6 h ahead controller predictions (dotted lines) and plant realizations (solid lines) of biogas production (black): the nominal controller (assuming nominal influent concentrations) systematically underestimates the prospective biogas production of the plant (taking elevated influent concentrations) and thereby slowly drives the system towards the upper GS filling limit. Initially, GS constraints can be ensured (magnification in GS plot) as the controller is informed on the true plant state at the beginning of each prediction horizon (state feedback). However, at around day 2.3, the GS soft constraint (grey dashed line) is violated for the first time, and on day 3.5, the GS constraint (black dashed line) is finally violated. By then, the controller still predicts decreasing GS filling levels (dotted line), but the plant in fact exceeds the maximum GS filling level soon after.

As state feedback was assumed, the unstable plant behavior also affects the controller predictions, underscored by the predicted constraint violations around day 3.7. If the optimization solver fails to determine a feasible solution, i.e., one that satisfies constraints, it reverts to solving an approximate problem with relaxed constraints (Qin and Badgwell, 2003). This approximate solution, though, cannot lead the system back into stable operation. Instead, by applying erratic substrate feedings, it fails to restore stability. Consequently, GS filling level, gas production, and pH assume clearly unstable or even unphysical values. In real life, such plant behavior should be prevented as it would require releasing or flaring off of excess biogas from the headspace, resulting in opportunity cost and avoidable greenhouse gas emissions. Remedies could be longer prediction horizons to better anticipate prospective GS constraint violations (Qin and Badgwell, 2003) or further limited maximum feed volume flows to restrict the erratic feeding.

By contrast, the robust multi-stage controller involves predictions of two different scenarios based on the two different realizations of the influent uncertainty, and thereby acts more conservatively. Mind the two-fold controller predictions in Fig. 6 (left), shown as dotted lines, particularly in the magnification. While for multi-stage MPC the cost function is evaluated for the average of the resulting scenarios, constraints must be satisfied for all scenarios. This is the reason why the robust MPC avoids feeding trajectories that result in hard and soft constraint violations of the upper GS filling limit, and therefore maintains stability despite the higher GS filling setpoint.

In general, however, the feeding pattern changed in favor of GrS compared with Sec. 3.3.2, even during stable operation of the nominal MPC. The main reason is that parameter was decreased by one order of magnitude (Tab. 2), and thus the relative importance of maintaining a stable GS filling level was highlighted. This corresponds with a relative increase in the importance of feed volume flows, Eq. (2.10). Note the different scales of the y-axis in the top subplots of Fig. 6 and the significantly lower OLR compared with Fig. 5. The second cost function summand in Eq. (2.10) penalizes absolute amounts of fed substrates. Given the mass-specific biogas potential of individual substrates (described by respective influent concentrations), it is plausible for the controller to opt for silage rather than manure to satisfy medium GS filling levels, and among silages, chooses GrS as the cheapest one available.

The increased robustness of multi-stage MPC comes at a price: the runtime is significantly longer than for nominal MPC, provided the solver does not need to revert to suboptimal solutions with constraint relaxation. This has been tested for the same scenario as discussed here, but with only 1 SD for influent uncertainty and a slightly reduced target filling level of 50% (plots shown in the SI). The total run time for nominal MPC was 263 s vs. 525 s for multi-stage MPC. Though compared to a simulated time of 14 d, multi-stage MPC is well real-time capable.

## 3.5 Limitations and outlook

The present results are based on simulations that assumed state feedback, i.e. ideal knowledge of the plant’s dynamic state. Moreover, the considered uncertainties were limited to influent macronutrients within known bounds. Further, disturbance feedings were considered predictable and of known uncertainty. Only agricultural substrates were considered, for which PR and LI were considered fully degradable. Lastly, independent feeding of five substrates was assumed, which is uncommon in full scale (Fachagentur Nachwachsende Rohstoffe e. V., 2021), albeit technically possible. Future research should thus address a state observer to estimate the process state from available measurements, experimental validation including non-agricultural substrates (e.g., organic wastes), and analysis of expected surplus revenues through flexible feeding.

# Conclusions

A robust multi-stage MPC framework was developed to optimize substrate feedings with uncertain influent macronutrients to an agricultural AD plant. In two case studies, the MPC delivered successful setpoint tracking of constant methane production and ensured safe GS capacity limits during demand-oriented CHP operation despite GS measurement noise. The robust MPC rejected disturbance feedings of especially high uncertainty and maintained process stability where nominal MPC resulted in plant failure. Simulation runtimes confirmed real-time capability. Future work should incorporate a state observer and address experimental validation.

# Supplementary Information

E-supplementary information of this work can be found in the online version of the paper.

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## Supplementary Figures

|  |
| --- |
| **(a)** |
| **(b)** |
| **(c)** |
| **Figure SI 1**: Sensitivity analysis of ADM1-R3 with respect to different influent macronutrient concentrations (a: CH, b: PR, c: LI) and effect on gas production and pH. Solid lines are based on elevated values (Simulator/Plant), and dotted lines on nominal values (Simulator 2), cf. Fig. 1d. |

|  |  |
| --- | --- |
|  |  |
| **Figure SI 2:** Comparison of robust (left) and nominal MPC (right) for cogeneration with lower target gas storage filling level and reduced influent uncertainty of only 1 SD. The prediction horizon was kept at 48 time steps (24 h). CHP on-times are indicated by grey background shading. | | |

## Supplementary Tables

**Table SI 1:** States, initial conditionsa and influent concentrationsb for ADM1-R3 (considering second carbohydrate fraction) and GSh. For macronutrients, resulting standard deviations are provided.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Index | Statec,f,g | Init.a,d | MSd,e,h | GrSd,e,h | SBSd,e,h | CMd,e,h |
| 1 |  | 0.05 | 10.32 | 10.44 | 8.17 | 4.54 |
| 2 |  | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 |
| 3 |  | 4.97 | 0.00 | 0.00 | 0.00 | 0.00 |
| 4 |  | 0.96 | 0.76 | 1.57 | 0.07 | 1.30 |
| 5 |  | 957.00 | 662.71 | 682.59 | 607.25 | 919.16 |
| 6 |  | 1.48 | 239.75±40.09 | 199.91±36.61 | 327.33±49.42 | 20.82±5.38 |
| 7 |  | 1.48 | 0.00 | 0.00 | 0.00 | 0.00 |
| 8 |  | 0.95 | 26.33±1.54 | 42.28±2.47 | 9.57±0.56 | 13.31±0.78 |
| 9 |  | 0.41 | 7.99±0.82 | 7.63±0.78 | 0.61±0.06 | 2.01±0.21 |
| 10 |  | 1.92 | 0.31 | 0.27 | 0.35 | 0.06 |
| 11 |  | 0.52 | 0.02 | 0.01 | 0.02 | 0.00 |
| 12 |  | 1.00 | 14.84 | 35.34 | 28.34 | 19.14 |
| 13 |  | 0.05 | -0.03 | 0.00 | 0.01 | 0.02 |
| 14 |  | 0.05 | 1.02 | 5.46 | 0.99 | 4.53 |
| 15 |  | 4.54 | 0.00 | 0.00 | 0.00 | 0.00 |
| 16 |  | 0.02 | 0.00 | 0.00 | 0.00 | 0.42 |
| 17 |  | 0.36 | 0.00 | 0.00 | 0.00 | 0.00 |
| 18 |  | 0.66 | 0.00 | 0.00 | 0.00 | 0.00 |
| 19 |  | 46 | - | - | - | - |
| 20 |  | 46 | - | - | - | - |
| - | pH | - | 3.8 | 4.8 | 4.9 | 8.54 |

a Initial conditions before transition into steady-state (SS). Dynamic simulations start from SS conditions (except and ).

b Influent concentrations are based on substrate characterization in Tab. 1 and further substrate analyses at DBFZ. Computations were done according to Delory et al. (2025).

c States 19 and 20 are only used in cogeneration case study. Given initial values are also used to initialize dynamic simulations.

d Concentrations in kg m-3 except in kmol m-3, and and in m3.

e pH of silages taken from Weißbach (2008), for manure from Fisgativa (2020).

f State 13 is the residual free ion concentration . Influent concentrations were computed via ionic states (14-16) and pH of substrates.

g Ionic states were assumed to be in dissociation equilibrium with their non-dissociated counterpart at the respective pH of the substrate.

h GS: gas storage, MS: maize silage, GrS: grass silage, SBS: sugar beet silage, CM: cattle manure

## Derivation of gas storage model equations

The volume flow of CH4 to the CHP unit can be derived via the specific gas constant of methane as

|  |  |  |
| --- | --- | --- |
|  |  | (0.1) |

Two additional states and describe the volume of CH4 and CO2 in the GS. An additional GS state for water could be avoided by assuming saturated vapor at . Under isobaric and isothermal conditions, mass balances simplify to volume balances

|  |  |  |
| --- | --- | --- |
|  |  | (0.2) |

The volume flow of CH4 required for a specific electrical CHP output entails the outflow of the remaining gases proportionate to their volume fraction within the GS

|  |  |  |
| --- | --- | --- |
|  | , | (0.3) |
|  | , | (0.4) |

where denotes the volume fraction of component (, , ) in the total GS volume. Inserting (0.4) into (0.3) delivers an expression independent of

|  |  |  |
| --- | --- | --- |
|  | . | (0.5) |

It was assumed that the volume flow from the AD process into the GS changes pressure and temperature instantaneously (from and to and ). Conservation of mass requires the outflow of the AD process to match the inflow into the GS. Applying the ideal gas law yields

|  |  |  |
| --- | --- | --- |
|  |  | (0.6) |

Inserting (0.6) into (0.2) delivers the ordinary differential equations (ODEs) of the two GS states

|  |  |
| --- | --- |
|  | (0.7) |
|  | (0.8) |